D-Phenylalanine 673-06-3 | DTXSID4025876

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Model Performance

Model	Data
Widdel	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		75%)	Test (25%	Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.85	0.69	0.86	0.67	0.86	0.78		

Model Results

Predicted value: -1.30

Global applicability domain: Inside

Local applicability domain index: 6.57e-01

Confidence level: 5.18e-01

Nearest Neighbors from the Training Set

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L-Phenylalanine Measured: -1.38 Predicted: -0.833

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Phenylalanine Measured: -1.38 Predicted: -0.833

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4-Fluoro-dl-phenylalanine Measured: -1.89 Predicted: -0.963

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Metaraminol
Measured: -0.270
Predicted: -0.842